SUPPLEMENTARY DATA

Effects of some anti-ulcer and anti-inflammatory natural products on cyclooxygenase and lipoxygenase enzymes: insights from *in silico* analysis

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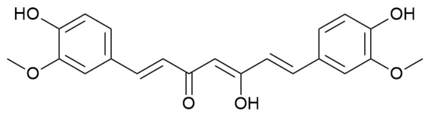
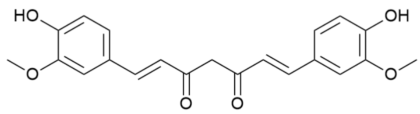
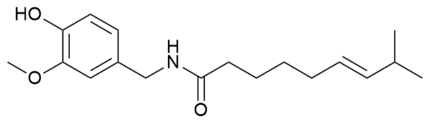
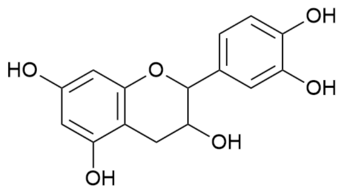
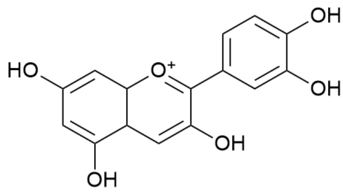
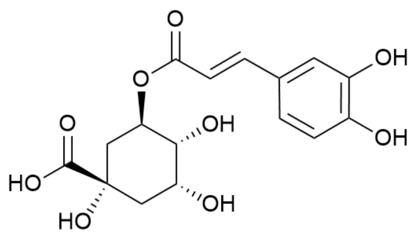
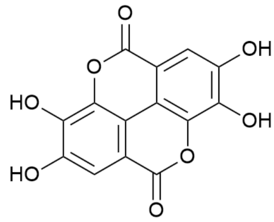
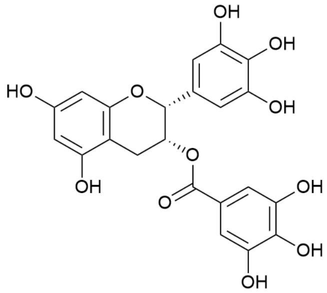
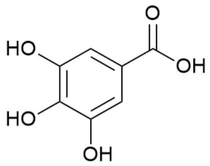
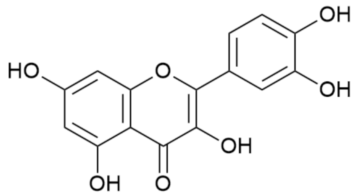
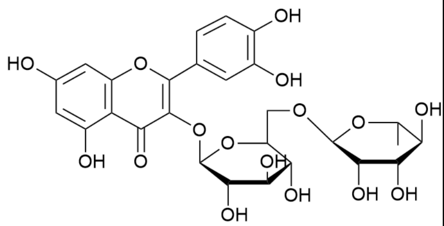
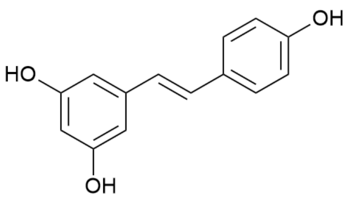
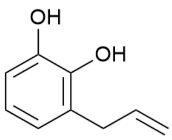
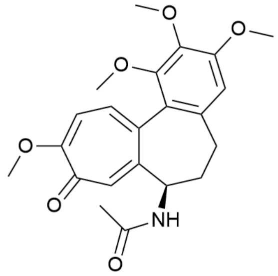
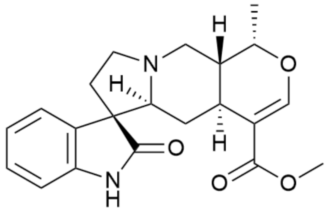
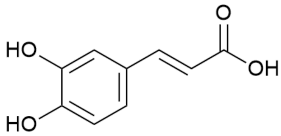
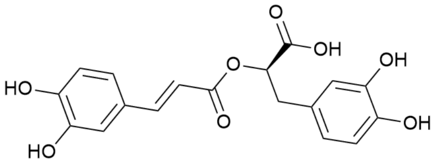
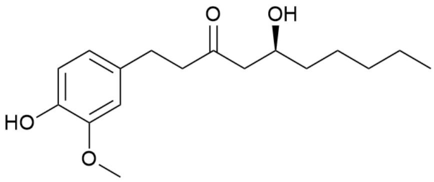
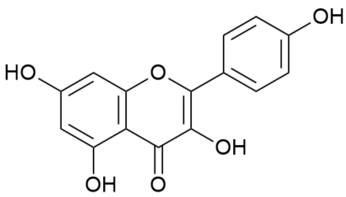
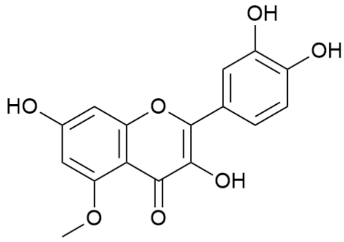
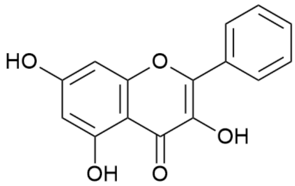
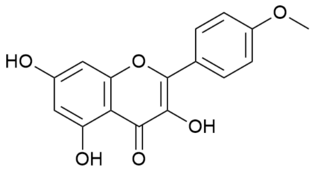
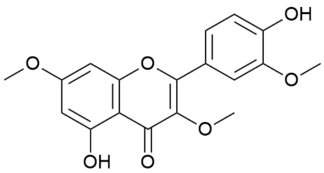
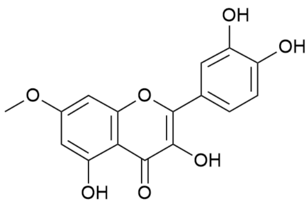
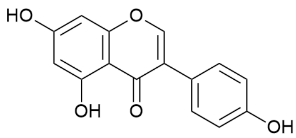
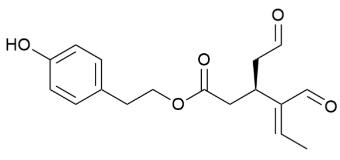
Table S1. The 31 phytochemicals with anti-inflammatory and anti-ulcer activities used in the docking studies.

S/N	Phytochemical	Structure	Plant source(s)	References
1	Curcumin	 Enol form  Keto form	*Curcuma longa* plants (Tumeric)	Tuorkey et al., 2009; Peng et al., 2021
2	Capsaicin		Chili peppers	Jolayemi et al., 2013
3	Catechin		Green tea (*Camellia sinensis*)	Kanoko et al., 2006 Singh et al., 2011
4	Cyanidin		red berries including grapes, bilberry, blackberry, blueberry, cherry, cranberry, elderberry, hawthorn, loganberry, açai berry and raspberry apples, pears, peaches and plums.	Zhang et al., 2020; Tian et al., 2020
5	Chlorogenic acid		Coffee, yerba mate, Eucommia ulmodies leaves, and Lonicerae Japonicae Flos	Bisht et al., 2020 Hwang et al., 2013

6	Ellagic acid		chestnuts, walnuts, pecans, cranberries, raspberries, strawberries, and grapes	Favarin et al., 2013
7	Epigallocatechin OR Epigallocatechin-3-gallate		*Green tea (Camellia sinensis) Black, white, and oolong tea*	Khalatbary et al., 2011; Wu et al., 2017; Singh et al., 2011
8	Gallic acid (3,4,5-trihydroxybenzoic acid)		gallnuts, sumac, witch hazel, tea leaves, oak bark	Kroes et al., 1992; Nouri et al., 2021
9	Quercetin		kal, apples, berries, red onions	Li et al., 2016; Saeedi-Boroujeni et al., 2021
11	Rutin (Quercetin-3-O-rutinoside)		Orange and lime leaves; *Carpobrotus edulis*	Jeong, 2009; Abdel-Raheem et al., 2010; Dubey et al., 2013
12	Resveratol OR 3,4′,5-Trihydroxy-*trans*-stilbene, 5-[(1*E*)-2-(4-Hydroxyphenyl)ethenyl]-1,3-benzenediol		Skin of grapes, blueberries, raspberries, mulberries, and peanuts	Salehi et al., 2018; Meng et al., 2021
13	Allylpyrocatecol OR (3-prop-2-enylbenzene-1,2-diol)		betel leaves	Sarkar et al., 2008

14	Colchicine		Autumn crocus (*Colchicum autumnale*)	Gasparyan et al., 2015
15	Mitraphylline		*Mitragyna speciosa Uncaria tomentosa*	Rojas-Duran et al., 2012
16	Caffeic acid		Coffee, *Elaeagnus augustifolia* bark of *Eucalyptus globulus*, barley grain, *Hordeum vulgare* and the herb *Dipsacus asperoides*	da Cunha et al., 2004; Zielińska et al., 2021
17	Rosmarinic acid		perilla, sweet basil, and rosemary	Marinho et al., 2021; Colica et al., 2018; Rocha et al., 2015
18	Gingerol		Ginger, tumeric	Shin et al., 2020; Mashhadi et al., 2013; Yamahara et al., 1988; Chioma et al., 2009
19	Kaempferol (3,4′,5,7-tetrahydroxyflavone)		Kale,apples, grapes, tomatoes, green tea, potatoes, onions, broccoli, cucumbers, lettuce, green beans, peaches, blackberries, raspberries, and spinach..	Zhang et al., 2020; Ekalu et al., 2020; Li et al., 2018; Wang et al., 2018

20	Azaleatin (quercetin 5-methyl ether) (2-(3,4-dihydroxyphenyl)-3,7-dihydroxy-5-methoxychromen-4-one)		flowers of *Rhododendron mucronatum* Rhododendron species.	Dai et al., 2021; Jazvinšćak Jembrek et al., 2021; Łyko et al., 2022
21	Galangin (3,5,7-trihydroxy-2-phenylchromen-4-one)		*Alpinia officinarum* (lesser galangal)	Thapa et al., 2023; Hassanein et al., 2023
22	Kaempferide (3,5,7-trihydroxy-2-(4-methoxyphenyl)chromen-4-one)		*Kaempferia galanga* (aromatic ginger)	Srivastava et al., 2019; Wang et al., 2021
23	Pachypodol (5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-3,7-dimethoxychromen-4-one)		*Pachypodanthium confine*, from leaves of *Agastache rugosa, (Korean mint)*, *Pogostemon cablin* Benth *Ballota* species	Fatima et al., 2023; Sever, 2002; Sever et al., 2006
24	Rhamnetin (2-(3,4-dihydroxyphenyl)-3,5-dihydroxy-7-methoxychromen-4-one)		clove (*Syzygium aromaticum*)	Jnawali et al., 2014; Batiha et al., 2020
25	Genistein		dyer's broom, *Genista tinctoria*;	Goh et al., 2022
26	Oleocanthal		Olive oil	Lucas et al., 2011

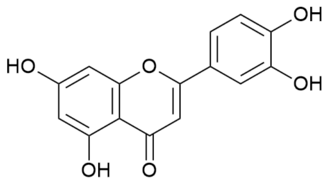
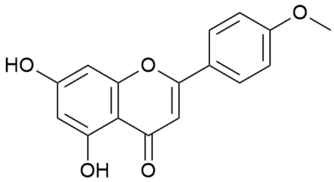
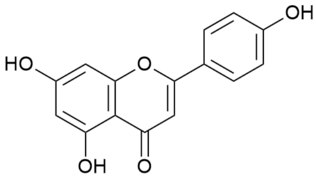
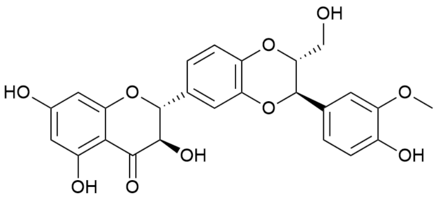
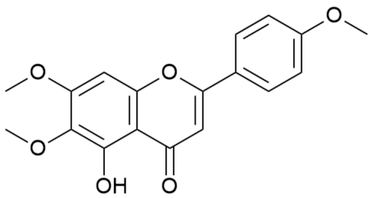
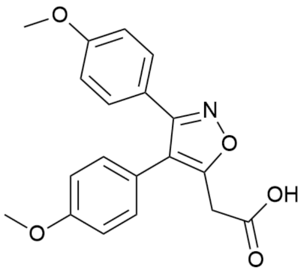
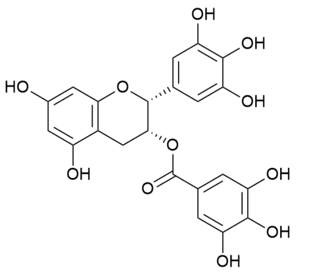
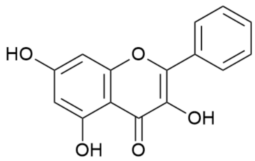
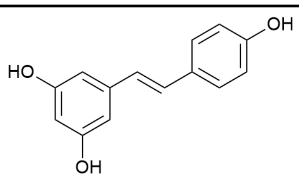
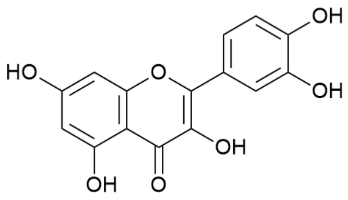
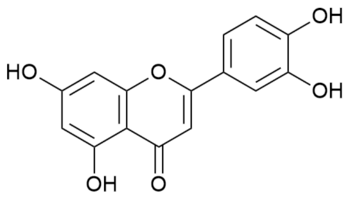
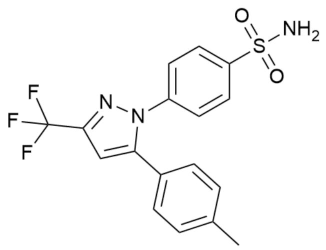
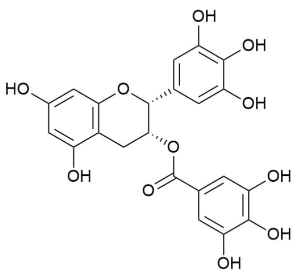
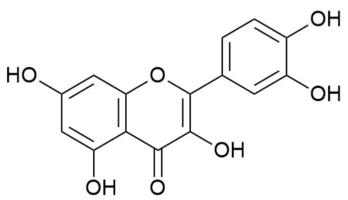
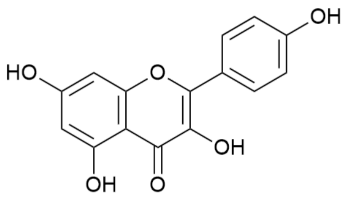
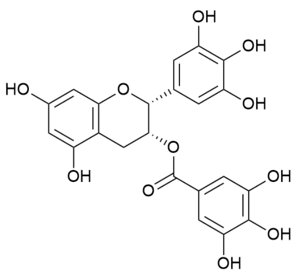
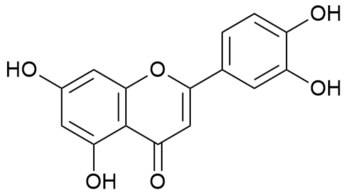
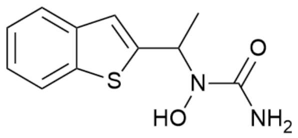
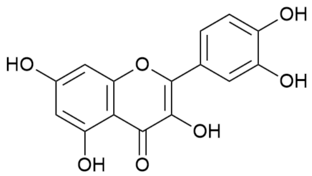
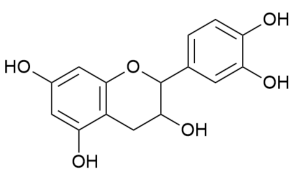
27	Luteolin (3′, 4′, 5, 7-tetrahydroxy-flavone)		*Reseda luteola*	Aziz et al., 2018; Conti et al., 2021
28	Acacetin		*Robiniapseudo acacia*	Carballo-Villalobos et al., 2014; Singh et al., 2020
29	Apigenin OR (4′, 5, 7-trihydroxyflavone),		parsley, celery, celeriac, and chamomile	Lee et al., 2007
30	Silymarin OR Silibinin		milk thistle plant	Alarcon et al., 1992; Lovelace et al., 2015; Tong et al., 2018
31	Salvigenin OR (5-Hydroxy-6,7,4'-trimethoxyflavone)		*Dorema glabrum* *Salvia officinalis*	Mansourabadi et al., 2016

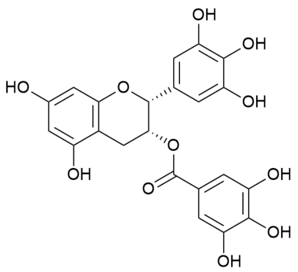
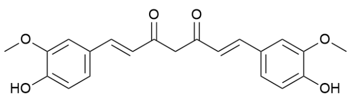
Table S2 Summary report of experimental data to show the effects of the most important reference compounds and phytochemicals on COX and LOX enzymes.

Cyclooxygenase-1 (COX-1)		
Compound	**Reported results**	**References**
 Mofezolac	● Most potent and selective reversible COX-1 inhibitor, fully inhibiting COX-1 and COX-2 with preference toward COX-1. ● It is used as a reference compound for docking towards COX-1. ● COX-1 IC_{50} = 0.0079 μM and COX-2 IC_{50} > 50 μM, with a selectivity index (SI) in favor of COX-1 higher than 6300].	Perrone et al., 2016; Cingolani et al., 2017; Pati et al.,. 2019
 Epigallocatechin-3-gallate	● Inhibits COX-1 activity to 96.9% at 50 μM, better than aspirin. ● Moderately blocks COX-1 (IC_{50} > 30 μM) but fails to significantly inhibit isolated COX-2 at 30 μM. ● Has a stronger effect than that of aspirin on inhibition of COX-1 activity.	Lee et al., 2013; Koeberle et al., 2009
 Galangin	● It showed both *in vitro* and *in vivo* to inhibit the catalytic activity of the COX-1/2 enzymes. ● Computational docking analysis together with quantum chemistry calculation shows that galangin can bind inside the peroxidase active sites of COX-1 and COX-2 in a similar manner as quercetin	Bai et al., 2021
 Resveratrol	● The compound inhibited the expression of both COX-1 and COX-2 proteins with IC_{50} ranging from 10 – 30 μM. ● The compound was found to be a potent peroxidase-mediated mechanism-based	Subbaramaiah et al., 1998; Szewczuk et al., 2004.

	inactivator of COX-1 only ($k_{\text{inact}} = 0.069 \pm 0.004\ \text{s}^{-1}$, $K_{i(\text{inact})} = 1.52 \pm 0.15\ \mu\text{M}$), with a calculated partition ratio of 22.	
 Quercetin  Luteolin	● Quercetin and luteolin showed strong inhibitory activities on 5-lipoxygenase (LOX), quercetin showing relatively potent inhibition on COX-1 reaction. ● Flavonoids possess inhibitory activity to COX-2 reaction, and especially luteolin, kaempferol, hesperetin, and naringin showed relatively potent inhibition on COX-2 reaction.	Lee and Kim, 2010
	Cyclooxygenase-2 (COX-2)	
 Celecoxib (Celebrex)	● Currently the only COX-2 inhibitor available in the U.S. ● Used as a reference compound for docking towards COX-2.	
 Epigallocatechin-3-gallate	● The compound was given by gavage, at a dose of 50 mg/kg body weight, and inhibited COX-2 expression in mice.	Kundu et al., 2003
 Quercetin	● Suppresses COX-2 expression by inhibiting the p300 signaling and blocking the binding of multiple trans activators to the COX-2 promoter.	Xiao et al.,

	● *In vitro* and *in vivo* studies show that quercetin suppresses COX-2 expression by inhibiting the p300 signaling and blocking the binding of multiple transactivators to the COX-2 promoter. ● The findings reveal a novel mechanism of action of quercetin and suggest a potential use for quercetin in the treatment of COX-2-mediated diseases such as breast cancers.	
 Kaempferol	● Effective against COX-2 at concentrations ranging 5 to 200 µmol/l). ● Kaempferol produced a significant concentration-dependent decrease of COX-2 protein level at all concentrations, but the percentage of inhibition induced by quercetin was reduced at high concentrations.	García-Mediavilla et al., 20
 Epigallocatechin-3-gallate	● Important constituent of green tea. Inhibits COX-2 expression ● The compound significantly inhibited constitutive COX-2 mRNA and protein overexpression. ● It was observed that the compound down-regulated the ERK1/2 and Akt pathways in colon cancer cells. ● Inhibition of COX-2 is a mechanism for the anti-proliferative effect of green tea and emphasizes the role that dietary factors have as anti-cancer agents.	Peng et al., 2006

 Luteolin	● Luteolin reduces the expression of inflammatory genes (iNOS and COX-2) and pro-inflammatory cytokines (TNF-α, IL-1β, and IL-6).	Huang et al., 2023.
Lipoxygenase (lipooxidase) (LOX-5)		
 Zileuton	● An FDA approved drug which is a 5-lipoxygenase (5-LOX) inhibitor. ● Selective inhibitor of LOX-5 with IC_{50} ranging from 0.1–9.1 µM). ● It is used as a reference compound for docking towards LOX-5. ● Zileuton IC_{50} for LOX-5 = 0.3 µM and PGE2 = 1.0 µM.	Kahnt et al., 2021
 Quercetin	● Inhibits 5-LOX with IC_{50} = 0.6 µmol/L ● A Comparison of the 5-LOX inhibitory effect of (−)-epicatechin with those of (−)-epigallocatechin gallate and quercetin showed (−)-epicatechin to be at least one order of magnitude more potent. ● IC_{50}, µmol/L ; (−)-Epicatechin = 22; (−)-Epigallocatechin gallate = 3.1; Quercetin = 0.6	Schewe et al., 2002
 Catechin	● Inhibits LOX-5 with IC_{50} ranging from 0.8 – 60 µmol/L ● Epicatechin and its related oligomers, the procyanidins caused dose-dependent inhibition of isolated rabbit 15-lipoxygenase-1 with the larger oligomers being more active; ● The decamer fraction revealed an IC_{50} of 0.8 µM. Among the monomeric flavanols,	Schewe et al., 2001

	epigallocatechin gallate (IC_{50} = 4 µM) and epicatechin gallate (5 µM) were more potent than (-)-epicatechin (IC_{50} = 60 µM). ● (-)-Epicatechin and procyanidin nonamer also inhibited the formation of 15-hydroxy-eicosatetraenoic acid from arachidonic acid in rabbit smooth muscle cells transfected with human 15-lipoxygenase-1.	
 Epigallocatechin-3-gallate	● X-ray analysis of the 3D structure of the compound interacting with soybean LOX-3 reveals the inhibitor depicting (-)-epigallo-catechin that lacks galloyl moiety. ● The A-ring is near the iron co-factor, attached by the H-bond to the C-terminus of the enzyme. ● The B-ring hydroxyl groups participate in the H-bonds and the van der Waals interactions formed by the surrounding amino acids and water molecules.	Skrzypczak-Jankun et al., 2003
 Curcumin	● Inhibited LOX and COX with IC_{50} values of 5-10 µM, ● Curcuminoids have shown significantly higher inhibitory effects on the peroxidase activity of COX-1 than that of COX-2. ● Curcumin and tetrahydrocannabinol potently inhibited the activity of human recombinant 5-LOX, showing estimated IC_{50} values of 0.7 and 3 µM, respectively.	Gadnayak et al., 2022 ; Hong et al., 2004; Huang et al., 1991.

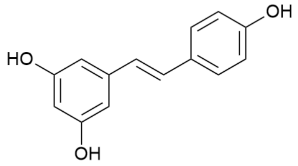
 Resveratrol	● Inhibits both COX-2 and 5-LOX enzymes. ● Molecular docking and molecular dynamics simulations have been used to design resveratrol derivatives for COX-2 and 5-LOX inhibition. ● By attaching several functional groups on four different places of the resveratrol scaffold, the R group enumeration approach was employed to build four libraries of resveratrol derivatives.	Doiphode et al., 2022

Table S3 Docking results, showing GScore values for the docked ligands and their most significant contributions towards COX-2

Compound	Gscore	E_{vdw}	E_{coul}	E_{lipo}	E_{hbond}	E_{rotb}	E_{site}	L_{eff}
Rutin	-14.04	-4.49	-10.96	-5.54	-6.20	16	-0.27	-0.33
Epigallocatechin-3-galla	-11.79	-11.11	-12.45	-5.23	-4.08	12	-0.4	-0.35
Quercetin	-11.16	-15.92	-10.68	-4.30	-4.12	6	0	-0.51
Rhamnetin	-10.55	-19.72	-5.64	-4.48	-3.79	6	0	-0.46
Azaleatin	-10.45	-26.42	-8.36	-4.77	-3.12	6	0	-0.45
Epigallocatechin	-9.92	-16.43	-11.90	-4.94	-2.63	7	0	-0.45
Ellagic acid	-9.64	-20.66	-5.53	-5.16	-2.4	4	0	-0.44
Pachypodol	-8.97	-40.87	-2.56	-5.86	-1.31	6	0	-0.36
Galangin	-8.48	-36.73	-4.10	-5.03	-0.67	4	0	-0.42
Curcumin-Enol	-9.77	-31.63	-9.61	-6.64	-1.44	10	-0.2	-0.31
Acacetin	-8.24	-32.69	-4.31	-5.05	-1.18	4	0	-0.39
Resveratol_-3,4,5-Trihy oxy-trans-stilbene-	-8.13	-26.34	-7.01	-4.89	-1.26	5	0	-0.48
Oleocanthal	-8.12	-27.74	-6.72	-5.03	-0.98	11	-0.64	-0.37
Curcumin-keto	-9.51	-28.79	-9.12	-6.32	-1.49	10	-0.26	-0.30
Gingerol	-7.96	-35.91	-6.08	-5.05	-1.43	12	-0.07	-0.38
Cyanidin (Neutral)	-8.25	-24.59	-7.92	-4.35	-2.06	3	-0.37	-0.38
Luteolin	-7.87	-35.47	-3.95	-4.86	-1.44	5	0	-0.37
Cyanidin (charged)	-7.68	-31.45	-8.13	-4.63	-1.12	6	0	-0.36
Kaempferide	-7.60	-35.77	-3.12	-5.12	-0.98	5	0	-0.34
Capsaicin	-7.34	-36.96	1.74	-5.54	-0.48	11	-0.35	-0.33
Catechin	-7.28	-33.29	-2.66	-4.92	-0.96	6	0	-0.34

Salvigenin	-7.06	-27.87	2.43	-4.87	-0.71	5	0	-0.29
Kaempferol	-7.04	-34.59	-2.97	-4.76	-0.96	5	0	-0.33
Genistein	-7.03	-24.35	-2.49	-4.93	-0.48	4	0	-0.35
Allylpyrocatecol-3-prop-enylbenzene-1,2-diol	-6.79	-21.41	-5.10	-3.86	-1.38	4	0	-0.62
Apigenin	-6.69	-33.32	-2.54	-4.76	-0.48	4	0	-0.33
Caffeic acid	-6.53	-20.15	-6.16	-3.30	-1.44	4	-0.33	-0.50
Gallic acid	-6.51	-20.40	-3.79	-2.79	-2.09	4	-0.4	-0.54
Chlorogenic acid	-5.73	-26.48	-0.39	-3.48	-2.88	10	-0.76	-0.23
Rosmarinic acid	-5.17	-29.86	-4.88	-4.33	-2.48	11	-0.36	-0.20
Celecoxib	-11.61	-50.31	-5.93	-6.67	-0.90	4	-1.16	-0.45

Table S4 Docking results, showing GScore values for the docked ligands and their most significant contributions towards 5-LOX

Compound	Gscore	E_{vdw}	E_{coul}	E_{lipo}	E_{hbond}	E_{rotb}	E_{site}	L_{eff}
Rutin	-11.12	-45.22	-23.54	-2.61	-6.74	16	0	-0.26
Salvigenin	-9.69	-30.85	-2.11	-3.39	-0.83	4	0	-0.37
Rosmarinic acid	-9.38	-21.39	-21.54	-1.13	-3.84	11	0	-0.36
Epigallocatechin-3-galla	-10.84	-32.54	-12.19	-2.65	-2.65	11	0	-0.28
Chlorogenic acid	-8.86	-18.65	-19.57	-0.94	-3.63	10	0	-0.35
Kaempferide	-7.151	-30.741	-4.766	-3.184	-2.11	5	0	-0.32
Silymarin	-6.98	-35.53	-14.37	-2.55	-3.35	9	0	-0.20
Galangin	-6.93	-27.91	-3.26	-3.27	-1.78	4	0	-0.34
Acacetin	-6.92	-26.63	-6.06	-3.22	-1.74	4	0	-0.33
Quercetin	-8.74	-22.74	-7.26	-2.14	-1.56	5	0	-0.31
Genistein	-6.88	-26.30	-6.15	-3.18	-1.75	4	0	-0.34
Cyanidin (Neutral)	-7.14	-23.92	-3.95	-1.41	-0.31	3	0	-0.32
Kaempferol	-6.83	-29.04	-3.90	-3.08	-1.96	5	0	-0.32
Apigenin	-8.48	-18.94	-5.08	-2.03	-1.57	3	0	-0.34
Rhamnetin	-9.33	-26.51	-10.05	-1.58	-2.70	5	0	-0.29
Epigallocatechin	-9.37	-21.54	-10.03	-1.27	-2.8	6	0	-0.31
Luteolin	-8.39	-19.94	-5.10	-2.07	-1.44	4	0	-0.32
Ellagic acid	-8.07	-25.67	-6.74	-1.63	-1.44	3	0	-0.30
Azaleatin	-9.14	-26.22	-4.24	-1.63	-1.75	5	0	-0.29
Salvigenin	-6.39	-33.81	-3.01	-3.35	-1.41	5	0	-0.27
Gingerol	-6.26	-24.67	-12.90	-2.35	-1.44	12	0	-0.30

Caffeic acid	-6.16	-10.58	-13.17	-0.74	-1.43	4	0	-0.47
Pachypodol	-6.12	-30.56	-8.31	-1.94	-2.20	6	0	-0.25
Cyanidin (charged)	-6.15	-22.46	-13.27	-2.08	-2.58	6	0	-0.30
Gallic acid	-5.91	-9.86	-11.20	-0.63	-1.44	4	0	-0.49
Arachidonic acid	-5.79	-20.26	-5.83	-2.37	0	14	0	-0.26
Catechin	-5.42	-24.46	-15.74	-1.24	-1.501	6	0	-0.26
Curcumin (Enol)	-6.81	-32.05	-11.47	-2.15	-2.53	10	0	-0.20
Capsaicin	-4.94	-28.40	-9.17	-2.28	-0.48	11	0	-0.22
Resveratol-3,4,5-Trihydxy-trans-stilbene	-4.92	-25.58	-3.28	-2.98	-0.20	5	0	-0.29
Colchicine	-4.83	-36.66	-4.02	-2.30	-1.06	6	0	-0.17
Oleocanthal	-4.65	-28.16	-12.77	-2.18	-1.03	11	0	-0.21
Curcumin (keto)	-6.02	-28.80	-10.14	-1.77	-2.21	10	0	-0.17
Mitraphylline	-4.09	-28.36	-2.82	-2.88	-0.73	2	0	-0.15
Allylpyrocatecol-3-propenylbenzene-1,2-diol	-3.92	-13.00	-11.90	-0.60	-1.92	4	0	-0.35
Celcoxib	-4.32	-30.78	-5.57	0	-0.73	4	0	-0.17
Zileuton	-7.85	-21.63	-6.88	0	0	3	0	-0.36

Table S5 Summary outputs from MM-GBSA calculations with free energies of binding (ΔG_{bind}) and free energies of solvation (ΔG_{solv}) of the selected compounds to the docked COX-2 protein target.

Compound	ΔG_{bind}	$\Delta G_{bind,vdw}$	$\Delta G_{bind,Coul}$	$\Delta G_{bind,hbond}$	$\Delta G_{bind,lipo}$	ΔG_{solv}	L_{strain}
Rutin	2.40	-1.61	-41.79	-4.44	-32.49	43.11	66.27
Epigallocatechin-3-gallate	-29.81	-22.33	-33.74	-3.37	-27.08	41.20	28.44
Quercetin	-47.64	-28.74	-27.62	-2.62	-19.45	22.29	11.49
Rhamnetin	-52.76	-29.89	-28.39	-2.17	-21.39	25.58	5.03
Azaleatin	-44.86	-28.64	-27.22	-2.71	-21.29	24.86	13.45
Epigallocatechin	-19.20	-12.60	-25.53	-1.70	-21.15	33.13	13.39
Ellagic acid	-41.69	-28.53	-14.75	-1.06	-20.26	17.68	8.89
Pachypodol	-52.32	-39.74	-17.70	-1.28	-26.07	20.54	14.00
Galangin	-53.55	-41.83	-20.02	-1.15	-22.23	25.27	7.68
Curcumin (enol form)	-43.81	-32.61	-22.80	-1.12	-31.77	27.92	26.74
Acacetin	-42.74	-29.45	-24.63	-1.30	-22.69	27.48	8.12
Resveratol-3,4,5-Trihydroxy-trans-stilbene-	-36.10	-26.99	-13.82	-1.63	-22.57	28.87	4.27
Oleocanthal	-22.97	-29.47	-10.87	-1.27	-23.02	26.65	26.09
Curcumin (keto form)	-33.59	-28.33	-22.51	-1.16	-30.74	31.29	28.40
Gingerol	-24.55	-23.83	-17.13	-1.28	-28.33	25.47	24.05
Cyanidin (neutral)	-20.83	-31.60	-49.96	-2.15	-13.32	73.35	5.22
Luteolin	-46.87	-36.51	-16.88	-1.45	-17.65	24.01	4.20
Cyanidin (charged)	-49.87	-33.37	92.37	-1.96	-15.41	-96.84	4.63

Kaempferide	-37.29	-34.08	-9.74	-0.70	-20.46	23.85	7.09
Capsaicin	-30.38	-32.60	-12.99	-0.49	-25.91	34.27	17.79
Catechin	-40.49	-35.80	-17.91	-0.91	-20.17	33.44	2.87
Salvigenin	-16.26	-22.18	-0.29	-1.02	-25.39	24.40	13.90
Kaempferol	-47.73	-36.84	-14.69	-1.38	-19.51	21.26	6.59
Genistein	-31.57	-28.21	-9.74	-0.71	-18.50	22.84	7.77
Allylpyrocatecol-3-prop-2-enylbenzene-1,2-diol-	-38.37	-25.35	-12.74	-0.88	-17.62	18.77	-0.29
Apigenin	-43.01	-37.53	-10.09	-1.16	-18.04	20.97	5.09
Caffeic acid	-21.61	-28.95	-24.36	-0.89	-16.42	47.11	1.75
Gallic acid	-10.75	-27.75	-11.65	-0.86	-12.26	41.75	0.31
Chlorogenic acid.	-6.87	-29.15	-4.20	-0.39	-22.46	41.54	8.49
Rosmarinic acid	-15.17	-35.32	-14.66	-1.86	-21.84	53.30	8.88
Celecoxib	-72.15	-56.26	-17.41	-2.70	-25.02	26.95	5.13

Table S6 Summary outputs from MM-GBSA calculations with free energies of binding (ΔG_{bind}) and free energies of solvation (ΔG_{solv}) of the selected compounds to the docked 5-LOX protein target.

Compound	ΔG_{bind}	$\Delta G_{bind,vdw}$	$\Delta G_{bind,Coul}$	$\Delta G_{bind,hbond}$	$\Delta G_{bind,lipo}$	ΔG_{solv}	L_{strain}
Rutin	-50.87	-41.17	-56.34	-4.042	-12.96	61.95	12.47
Salvigenin	-31.25	-36.88	-128.95	-0.89	-16.88	153.03	7.68
Rosmarinic acid	-46.80	-26.68	-53.82	-2.66	-7.84	45.51	9.19
Epigallocatechin-3-gallate	-20.56	-33.28	-147.56	-1.92	-9.03	156.95	17.85
Chlorogenic acid	-44.91	-23.19	-98.32	-1.66	-10.04	81.79	6.47
Kaempferide	-40.88	-30.25	-23.59	-1.90	-17.77	35.49	4.70
Silymarin (Silibinin)	-30.81	-40.98	-23.70	-2.24	-12.40	42.14	6.02
Galangin	-31.44	-29.28	-17.68	-1.38	-16.78	36.68	3.99
Acacetin	-34.75	-29.50	-10.71	-1.28	-18.09	24.67	5.26
Quercetin	-27.36	-21.48	-168.10	-1.59	-9.88	170.59	6.06
Genistein	-27.78	-25.59	-13.16	-2.22	-16.12	31.25	7.56
Cyanidin (neutral)	-30.51	-25.27	-90.27	-0.93	-4.37	90.64	1.28
Kaempferol	-40.25	-27.77	-22.58	-2.01	-17.07	31.49	4.33
Apigenin	-24.54	-22.69	-153.55	-0.80	-9.40	163.79	1.46
Rhamnetin	-33.54	-28.53	-132.40	-1.95	-7.15	135.36	3.32
Epigallocatechin	-32.78	-19.37	-159.05	-1.71	-5.47	151.56	-0.46
Luteolin	-26.09	-23.43	-149.66	-0.85	-9.42	159.15	0.79
Ellagic acid	-29.98	-25.19	-152.67	-1.24	-9.36	160.51	1.57
Azaleatin	-22.43	-28.13	-115.25	-1.71	-6.34	128.58	2.73

Salvigenin	-39.39	-36.19	-16.05	-0.88	-18.77	37.08	3.97
Gingerol	-11.25	-26.51	-18.36	-0.61	-8.83	45.33	11.66
Caffeic acid	-34.87	-12.02	-72.82	-1.34	-5.28	56.28	0.45
Pachypodol	-27.41	-32.02	-12.75	-1.75	-14.40	29.81	5.63
Cyanidin (charged)	-33.12	-23.09	102.33	-2.30	-7.64	-102.51	4.64
Gallic acid	-34.30	-11.91	-73.98	-1.28	-4.69	57.58	0.98
Arachidonic acid	-45.06	-32.45	-38.98	-0.02	-13.14	37.08	5.64
Catechin	-30.45	-26.29	-27.02	-3.04	-11.54	39.43	2.71
Curcumin (enol form)	-29.08	-39.20	-26.80	-2.20	-11.66	47.61	10.96
Capsaicin	-19.19	-35.22	-13.38	-1.03	-13.38	42.71	10.07
Resveratol-3,4,5-Trihydroxy-trans-stilbene	-24.05	-27.12	-19.69	-1.21	-17.34	40.72	5.08
Colchicine	-29.88	-34.36	-13.64	-1.56	-16.74	34.88	5.12
Oleocanthal	-25.63	-31.96	-16.38	-1.18	-10.06	33.33	7.16
Curcumin (keto form)	-28.74	-40.20	-19.72	-0.95	-12.40	43.91	2.12
Mitraphylline	-29.64	-29.94	25.91	-0.75	-13.25	-11.97	4.00
Allylpyrocatecol_-3-prop-2-enylbenzene-1,2-diol	-18.79	-15.66	-21.73	-1.16	-7.89	28.32	2.03
Celecoxib	-27.35	-36.51	-6.61	-1.75	-12.67	31.14	3.76
Zileuton	-40.37	-22.27	-75.85	-1.31	-7.19	65.01	2.56

Table S7. Per-residue interaction energies for selected docked poses of the phytochemicals against the target proteins and breakdown of interaction energies into van der Waals and electrostatic interactions.

Name	**Forcefield**	**Total Interaction Energy (kcal/mol)**	**Total VDW Interaction Energy (kcal/mol)**	**Total Electrostatic Interaction Energy (kcal/mol)**
5-LOX_Rosmarinic_acid _model_1	cff	-85.68397	-11.21658	-74.46739

Interaction Energies			
Residue	**Interaction Energy (kcal/mol)**	**VDW Interaction Energy (kcal/mol)**	**Electrostatic Interaction Energy (kcal/mol)**
Trp147	-0.081688	-0.034127	-0.047561
Phe151	-0.219583	-0.017168	-0.202414
His160	-0.033514	-0.055131	0.021617
Phe169	-0.629543	-0.495275	-0.134268
Asp170	4.788596	-0.032117	4.820713
Ser171	-0.223176	-0.121078	-0.102098
Phe177	-14.386240	-2.895304	-11.490936
Val178	-0.128142	-0.082815	-0.045327
Leu179	-0.447615	-0.093377	-0.354238
Asn180	-1.299070	-0.338547	-0.960523
Tyr181	-0.140932	-0.040147	-0.100785
Lys183	-5.587302	-0.041490	-5.545812
Ala240	0.098951	-0.024256	0.123207
Phe359	-0.084190	-0.208293	0.124103
His360	0.334502	-0.062686	0.397188
Val361	0.183653	-0.027745	0.211398
His362	-0.276877	-0.260715	-0.016162
Gln363	0.921512	2.640118	-1.718606
Thr364	0.159265	-0.193977	0.353242
Ile365	0.226665	-0.047033	0.273699
Thr366	0.052497	-0.056214	0.108712
His367	-2.429813	-3.390910	0.961097
Leu368	-0.773902	-0.822161	0.048258
Leu369	0.223847	-0.052284	0.276131
Thr371	-0.306722	-0.151843	-0.154879
His372	-0.057959	-1.280529	1.222570
Leu373	-0.124097	-0.075029	-0.049068
Ser375	-0.564589	-0.030902	-0.533687
Glu376	6.726786	-0.039734	6.766519
His399	-0.006226	-0.017835	0.011609
Phe402	0.037765	-0.139018	0.176782

Thr403	0.292654	-0.154413	0.447067
Ile404	0.328580	-0.055784	0.384364
Ala405	0.003710	-0.132745	0.136455
Ile406	-3.420168	-3.605201	0.185033
Asn407	1.142123	-0.481834	1.623956
Thr408	-0.166591	-0.090639	-0.075951
Lys409	-8.385477	-0.778315	-7.607162
Ala410	-1.440141	-0.908453	-0.531688
Arg411	-7.257557	-0.110521	-7.147036
Glu412	6.236320	-0.064669	6.300988
Gln413	0.083392	-0.207014	0.290405
His432	-0.021451	-0.081831	0.060380
Met435	-0.128745	-0.014213	-0.114532
Val436	-0.143902	-0.018784	-0.125118
Thr545	0.261902	-0.022030	0.283932
Ala546	0.298345	-0.042967	0.341312
Ser547	0.360205	-0.028957	0.389162
Gln549	-0.122727	-0.031843	-0.090884
His550	0.641591	-1.184985	1.826577
Ala551	0.254161	-0.075333	0.329494
Ala552	0.035555	-0.025530	0.061085
Val553	-0.125483	-0.151597	0.026115
Asn554	-0.134371	-1.982677	1.848306
Phe555	-0.661795	-0.878260	0.216464
Gly556	-0.237995	-0.031976	-0.206019
Gln557	-2.917215	-1.578042	-1.339174
Tyr558	-0.168179	-0.066769	-0.101410
Ala561	-0.169997	-0.029971	-0.140026
Ala567	0.048359	-0.012827	0.061186
Pro569	-0.053101	-0.034043	-0.019059
Trp599	0.106367	-0.025046	0.131413
His600	0.127543	-0.050109	0.177652
Ala603	-0.094016	-0.177327	0.083312
Val604	-0.049778	-0.272442	0.222665
Trp605	0.134721	-0.061967	0.196688
Ala606	-0.215725	-0.121905	-0.093821
Leu607	-3.397986	-3.198517	-0.199469
Ser608	0.019616	-0.123744	0.143360
Gln609	-0.025262	-0.128748	0.103486
Phe610	-0.697763	-0.845237	0.147475
Glu614	1.641288	-0.156825	1.798112
Arg666	-4.671966	-0.022888	-4.649077
Pro668	-0.284888	-0.117278	-0.167610
Asn669	-0.018427	-0.023584	0.005158
Ser670	-0.044424	-0.156831	0.112407
Val671	0.327561	0.834506	-0.506945
Ala672	-1.440793	-2.075413	0.634621

Fe2701	-59.664654	3.529543	-63.194195
UNK900	12.179750	13.347076	-1.167327

Name	Forcefield	Total Interaction Energy (kcal/mol)	Total VDW Interaction Energy (kcal/mol)	Total Electrostatic Interaction Energy (kcal/mol)
5-LOX_Rutin_model_1	cff	-66.67785	-16.81687	-49.86099

Interaction Energies			
Residue	**Interaction Energy (kcal/mol)**	**VDW Interaction Energy (kcal/mol)**	**Electrostatic Interaction Energy (kcal/mol)**
Trp147	-0.114758	-0.103812	-0.010946
Asn148	0.000241	-0.013738	0.013979
Phe151	-0.022976	-0.042113	0.019137
His160	-0.129253	-0.112727	-0.016525
Leu163	-0.023559	-0.023702	0.000142
Phe169	-0.556751	-0.545656	-0.011095
Asp170	0.250975	-0.065710	0.316685
Ser171	-0.452293	-0.399833	-0.052460
Phe177	-10.807402	-6.349091	-4.458310
Val178	-0.557551	-0.489534	-0.068017
Leu179	-1.890626	-1.574001	-0.316626
Asn180	-3.011028	-3.060351	0.049323
Tyr181	-0.263530	-0.208594	-0.054936
Ser182	-0.211020	-0.095938	-0.115082
Lys183	-2.403264	-1.278775	-1.124489
Ala184	-0.113411	-0.084992	-0.028418
Met185	-0.056963	-0.024908	-0.032055
Glu186	0.159768	-0.021254	0.181021
Asn187	-0.060817	-0.059555	-0.001262
Ala240	0.010027	-0.024992	0.035019
Asn241	0.005716	-0.022917	0.028633
Phe304	-0.004955	-0.015465	0.010511
Asp358	-0.257106	-0.016587	-0.240519
Phe359	-0.268963	-0.191576	-0.077386
His360	-0.235891	-0.095286	-0.140605
Val361	-0.061396	-0.046366	-0.015030
His362	-0.438503	-0.361560	-0.076943
Gln363	-4.023634	-2.447541	-1.576093
Thr364	-0.463185	-0.482836	0.019651
Ile365	-0.061734	-0.093650	0.031915
Thr366	-0.056137	-0.087472	0.031335
His367	-2.166901	-2.229704	0.062804
Leu368	-2.646520	-2.613849	-0.032670
Leu369	-0.073812	-0.101263	0.027451

Arg370	-0.040407	-0.042621	0.002214
Thr371	-0.173003	-0.155342	-0.017661
His372	-2.302449	-2.726434	0.423986
Leu373	-0.120986	-0.132887	0.011901
Ser375	-0.053533	-0.032350	-0.021183
Glu376	-0.104349	-0.054451	-0.049898
His399	-0.019405	-0.018222	-0.001183
Phe402	-0.131841	-0.142953	0.011112
Thr403	-0.162778	-0.157725	-0.005053
Ile404	-0.098363	-0.076481	-0.021882
Ala405	-0.276390	-0.217059	-0.059331
Ile406	-3.603322	-2.862995	-0.740328
Asn407	-0.795206	-0.749671	-0.045535
Thr408	-0.249616	-0.229638	-0.019978
Lys409	-3.166902	-2.646281	-0.520621
Ala410	-2.513090	-2.611406	0.098316
Arg411	-0.219136	-0.379462	0.160327
Glu412	0.104472	-0.232459	0.336931
Gln413	-0.988799	-1.318777	0.329978
Gly430	0.358911	-0.009604	0.368516
His432	-0.153850	-0.178432	0.024582
Val433	-0.037312	-0.030205	-0.007107
Met435	-0.005070	-0.027364	0.022294
Val436	-0.019383	-0.044328	0.024945
Thr545	0.002054	-0.022649	0.024704
Ala546	-0.025380	-0.040279	0.014900
Ser547	0.002837	-0.027416	0.030254
Gln549	-0.024339	-0.032768	0.008429
His550	-0.281922	-0.767838	0.485916
Ala551	-0.021381	-0.068932	0.047551
Ala552	-0.027874	-0.025224	-0.002650
Val553	-0.172919	-0.157573	-0.015346
Asn554	-0.878694	-1.461911	0.583217
Phe555	-0.617925	-0.710440	0.092515
Gly556	-0.072963	-0.030539	-0.042424
Gln557	-1.591146	-1.070760	-0.520387
Tyr558	-0.090435	-0.081924	-0.008511
Ala561	-0.023864	-0.026102	0.002238
Pro569	-0.041043	-0.039179	-0.001864
His600	-0.064152	-0.059410	-0.004742
Gly602	-0.078800	-0.062564	-0.016236
Ala603	-0.310042	-0.303347	-0.006694
Val604	-0.294444	-0.258425	-0.036018
Trp605	-0.305216	-0.204842	-0.100374
Ala606	-1.281348	-0.670416	-0.610932
Leu607	-5.629145	-5.463543	-0.165602
Ser608	-0.370639	-0.301315	-0.069324

Gln609	-2.025838	-0.864218	-1.161620
Phe610	-1.714667	-1.599136	-0.115531
Glu614	-0.110917	-0.160369	0.049451
Pro668	-0.107958	-0.103643	-0.004315
Asn669	-0.021093	-0.023259	0.002166
Ser670	-0.141112	-0.139146	-0.001966
Val671	-0.748323	0.359925	-1.108248
Ala672	-2.209702	-2.308291	0.098590
Fe2701	-9.491151	3.120060	-12.611211
UNK900	7.870703	35.251102	-27.380400

Name	**Forcefield**	**Total Interaction Energy (kcal/mol)**	**Total VDW Interaction Energy (kcal/mol)**	**Total Electrostatic Interaction Energy (kcal/mol)**
COX-2_Kaempferol_model_1	cff	-67.15215	-17.09410	-50.05805

Interaction Energies			
Residue	**Interaction Energy (kcal/mol)**	**VDW Interaction Energy (kcal/mol)**	**Electrostatic Interaction Energy (kcal/mol)**
Pro86	-0.087327	-0.104881	0.017554
Asn87	-0.016658	-0.098665	0.082007
Thr88	-0.007143	-0.021760	0.014617
Val89	-0.090957	-0.091078	0.000121
His90	1.200811	1.507182	-0.306371
Tyr91	-0.030275	-0.053771	0.023496
Ile92	-0.028292	-0.024708	-0.003584
Leu93	-0.229103	-0.192722	-0.036381
Thr94	-0.284755	-0.230604	-0.054150
His95	-0.043660	-0.025499	-0.018162
Ile112	-0.016410	-0.018343	0.001933
Met113	-0.065559	-0.075228	0.009669
Val116	-0.208259	-0.210201	0.001941
Leu117	-0.073804	-0.081438	0.007634
Ser119	-0.029436	-0.025581	-0.003854
Arg120	-1.191208	-0.873714	-0.317494
Ser121	-0.045651	-0.031286	-0.014365
Ile124	-0.020184	-0.024148	0.003964
Asp190	-0.399115	-0.060737	-0.338378
Pro191	-0.014210	-0.035749	0.021540
Gln192	-1.471097	-1.043553	-0.427545
Gly193	-0.001773	-0.011238	0.009466
Ser194	-0.009761	-0.035990	0.026229
Phe198	-0.215390	-0.204143	-0.011247
Phe201	-0.043352	-0.039930	-0.003422
Ala202	-0.060880	-0.046084	-0.014796
Phe205	-0.066684	-0.103792	0.037108

Thr206	-0.035989	-0.056983	0.020994
Phe209	-0.012273	-0.041578	0.029304
Phe210	-0.029654	-0.035715	0.006061
Val228	-0.005795	-0.011481	0.005685
Ile341	-0.033370	-0.027869	-0.005501
Ile343	-0.020914	-0.027894	0.006981
Val344	-0.248034	-0.263387	0.015353
Ile345	-0.251696	-0.246980	-0.004716
Glu346	-0.018273	-0.049197	0.030924
Asp347	-0.073286	-0.059283	-0.014002
Tyr348	-0.985116	-1.036754	0.051638
Val349	-3.179230	-3.201512	0.022281
Asn350	-0.354171	-0.368792	0.014621
His351	-0.311350	-0.350600	0.039250
Leu352	-3.833032	-3.937166	0.104134
Ser353	-3.493294	-3.531005	0.037710
Gly354	-0.242580	-0.354708	0.112128
Tyr355	-2.583024	-2.571122	-0.011902
His356	-0.047283	-0.035941	-0.011343
Phe357	-0.074695	-0.075860	0.001164
Lys358	-0.072680	-0.026104	-0.046576
Leu359	-0.547104	-0.538517	-0.008587
Lys360	-0.058307	-0.022968	-0.035339
Phe381	-0.241678	-0.270673	0.028995
Asn382	-0.018531	-0.014843	-0.003687
Leu384	-0.189321	-0.190889	0.001568
Tyr385	-1.385528	-1.103167	-0.282361
Trp387	-0.763186	-0.606561	-0.156625
Leu390	-0.029203	-0.034310	0.005106
Arg433	0.211535	-0.049663	0.261198
Val434	-0.028723	-0.068494	0.039771
Ala435	-0.029857	-0.042701	0.012844
Leu472	-0.031400	-0.027015	-0.004385
Leu507	-0.039417	-0.038639	-0.000778
Glu510	0.046319	-0.043616	0.089935
Lys511	-0.105942	-0.033574	-0.072368
Pro512	-0.048035	-0.087760	0.039725
Arg513	-2.796485	-1.723152	-1.073333
Pro514	-0.104421	-0.121850	0.017429
Asp515	-0.077722	-0.093398	0.015676
Ala516	0.661015	0.337249	0.323766
Ile517	-0.803612	-0.992151	0.188540
Phe518	-3.155260	-3.281177	0.125917
Gly519	-0.332349	-0.346943	0.014593
Glu520	0.048918	-0.250452	0.299370
Thr521	-0.074388	-0.095529	0.021141
Met522	-0.635086	-0.616144	-0.018942

Val523	-2.544914	-2.423049	-0.121864
Glu524	-0.130896	-0.489096	0.358200
Val525	-0.169972	-0.156969	-0.013003
Gly526	-1.149152	-1.074931	-0.074221
Ala527	-3.306024	-3.315668	0.009645
Pro528	-0.349112	-0.359031	0.009919
Phe529	-0.207568	-0.226073	0.018506
Ser530	0.197617	0.970584	-0.772966
Leu531	-1.785067	-1.684704	-0.100363
Lys532	-0.025262	-0.057962	0.032700
Gly533	0.001614	-0.027008	0.028622
Leu534	-0.274061	-0.266157	-0.007903
Met535	-0.038043	-0.029004	-0.009039
UNK900	-27.387674	20.969498	-48.357174

Name	**Forcefield**	**Total Interaction Energy (kcal/mol)**	**Total VDW Interaction Energy (kcal/mol)**	**Total Electrostatic Interaction Energy (kcal/mol)**
COX-2_Rhamnetin_model_1	cff	-36.56216	-2.08042	-34.48175

Interaction Energies			
Residue	**Interaction Energy (kcal/mol)**	**VDW Interaction Energy (kcal/mol)**	**Electrostatic Interaction Energy (kcal/mol)**
Pro86	-0.083592	-0.105331	0.021739
Asn87	-0.008957	-0.098228	0.089271
Val89	-0.128616	-0.104330	-0.024286
His90	-1.527792	-1.475798	-0.051993
Tyr91	-0.043208	-0.054144	0.010936
Ile92	-0.044881	-0.027277	-0.017604
Leu93	-0.287109	-0.248219	-0.038890
Thr94	-0.288534	-0.223528	-0.065006
His95	-0.044493	-0.027273	-0.017221
Ile112	-0.012584	-0.025258	0.012674
Met113	-0.095823	-0.114311	0.018488
Tyr115	-0.022295	-0.034660	0.012365
Val116	-0.359153	-0.377446	0.018293
Leu117	-0.094138	-0.118444	0.024306
Thr118	-0.001007	-0.018161	0.017154
Ser119	-0.037024	-0.034057	-0.002967
Arg120	-1.994431	-1.257333	-0.737098
Ser121	-0.055928	-0.038312	-0.017616
Ile124	-0.025202	-0.026132	0.000931
Asp190	-0.831511	-0.115787	-0.715725
Pro191	-0.025839	-0.060836	0.034997
Gln192	-2.380816	-1.085544	-1.295272
Gly193	-0.011178	-0.016078	0.004899

Ser194	-0.001544	-0.052000	0.050455
Phe198	-0.191339	-0.203087	0.011748
Phe201	-0.026031	-0.040227	0.014195
Ala202	-0.022682	-0.040793	0.018112
Phe205	-0.092084	-0.114706	0.022622
Thr206	-0.023707	-0.054009	0.030301
Phe209	-0.030508	-0.043951	0.013443
Phe210	-0.027461	-0.033685	0.006224
Val228	-0.013035	-0.012579	-0.000456
Ile341	-0.031216	-0.031621	0.000405
Ile343	-0.033037	-0.030490	-0.002547
Val344	-0.318614	-0.301964	-0.016649
Ile345	-0.309503	-0.296229	-0.013274
Glu346	-0.006669	-0.057392	0.050722
Asp347	-0.149435	-0.065144	-0.084291
Tyr348	-1.101425	-1.016346	-0.085079
Val349	-2.252239	-2.178105	-0.074135
Asn350	-0.409964	-0.421377	0.011413
His351	-0.436405	-0.428741	-0.007663
Leu352	-1.330981	-1.527989	0.197009
Ser353	-4.148324	-4.310426	0.162102
Gly354	-0.299832	-0.390447	0.090615
Tyr355	-1.816566	-1.291562	-0.525004
His356	-0.067488	-0.041276	-0.026212
Phe357	-0.110095	-0.099891	-0.010204
Lys358	-0.039878	-0.032521	-0.007358
Leu359	-0.774906	-0.760046	-0.014859
Lys360	-0.101871	-0.029665	-0.072207
Phe381	-0.290362	-0.277936	-0.012426
Leu384	-0.163906	-0.154468	-0.009439
Tyr385	-0.936837	-0.824835	-0.112003
Trp387	-0.949647	-0.958630	0.008983
Leu390	-0.032193	-0.039792	0.007599
Gly432	-0.038738	-0.012405	-0.026333
Arg433	0.314912	-0.089758	0.404670
Val434	-0.079171	-0.101971	0.022801
Ala435	-0.102221	-0.075803	-0.026418
Gly436	-0.021507	-0.009116	-0.012391
Leu507	-0.030364	-0.042606	0.012243
Glu510	0.185373	-0.054595	0.239968
Lys511	-0.010323	-0.043620	0.033297
Pro512	-0.115101	-0.135585	0.020485
Arg513	-3.874628	-2.133211	-1.741417
Pro514	-0.211073	-0.136657	-0.074416
Asp515	-0.508659	-0.139005	-0.369655
Ala516	2.728384	2.267915	0.460468
Ile517	1.690459	1.020576	0.669883

Phe518	-2.019594	-1.134727	-0.884867
Gly519	-0.290349	-0.482039	0.191690
Glu520	0.169075	-0.270764	0.439839
Thr521	-0.074981	-0.099489	0.024509
Met522	-0.701628	-0.596787	-0.104841
Val523	-2.701875	-2.545788	-0.156086
Glu524	0.113051	-0.505375	0.618426
Val525	-0.146957	-0.150428	0.003470
Gly526	-0.975957	-1.013683	0.037726
Ala527	-3.347826	-3.317930	-0.029896
Pro528	-0.360589	-0.393126	0.032537
Phe529	-0.225368	-0.237066	0.011698
Ser530	3.786999	3.753637	0.033362
Leu531	-0.700639	-0.645249	-0.055390
Lys532	-0.194660	-0.065646	-0.129013
Gly533	-0.041080	-0.030206	-0.010875
Leu534	-0.333285	-0.305961	-0.027324
Met535	-0.053475	-0.035040	-0.018434
Phe580	-0.066172	-0.048405	-0.017768
UNK900	-3.380301	27.577913	-30.958214

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